

Exhibit 1

Molecules To Go (NIH)

(Formerly known as Molecules R Us)

Request an image of a PDB file "the way you want it"!.

Instructions | PDB Search Form | NIH Home Page

Viewers provide interactive molecules, and require the appropriate helper application. Image selections provide static "gif" images, and Java options provide inline interactive displays.]

Viewing Molecule: Output Requested:

Parameters effect Static Image generation only:

Image to be generated by Rasmol (fast) or Raster3D (slow)

Color by: (* => *Rasmol only*)

Rotations (0 - 360) degrees (for image only)

X-Axis: Y-Axis: Z_Axis:

First 100 lines from the PDB structure record... 1crl... Filesize = 109877

HEADER	HYDROLASE (CARBOXYLIC ESTERASE)	02-MAR-93	1CRL	1CRL	2
COMPND	LIPASE (E.C.3.1.1.3) (TRIACYLGLYCEROL HYDROLASE)			1CRL	3
SOURCE	FUNGUS (CANDIDA RUGOSA) (FORMERLY CYLINDRACEA)			1CRL	4
AUTHOR	P.GROCHULSKI,M.CYGLER			1CRL	5
REVDAT	1 31-JAN-94 1CRL 0			1CRL	6
JRNL	AUTH P.GROCHULSKI,Y.LI,J.D.SCHRAG,F.BOUTHILLIER,P.SMITH,			1CRL	7
JRNL	AUTH 2 D.HARRISON,B.RUBIN,M.CYGLER			1CRL	8
JRNL	TITL INSIGHTS INTO INTERFACIAL ACTIVATION FROM AN			1CRL	9
JRNL	TITL 2 'OPEN' STRUCTURE OF CANDIDA RUGOSA LIPASE			1CRL	10
JRNL	REF J.BIOL.CHEM. V. 268 12843 1993			1CRL	11
JRNL	REFN ASTM JBCHA3 US ISSN 0021-9258	071		1CRL	12
REMARK	1			1CRL	13
REMARK	1 REFERENCE 1			1CRL	14
REMARK	1 AUTH Y.KAWAGUCHI,H.HONDA,J.TANIGUCHI-MORIMURA,S.IWASAKI			1CRL	15
REMARK	1 TITL THE CODON CUG IS READ AS SERINE IN AN ASPOROGENIC			1CRL	16
REMARK	1 TITL 2 YEAST CANDIDA CYLINDRACEA			1CRL	17
REMARK	1 REF NATURE v. 341 164 1989			1CRL	18
REMARK	1 REFN ASTM NATUAS UK ISSN 0028-0836	006		1CRL	19
REMARK	2 RESOLUTION. 2.06 ANGSTROMS.			1CRL	20
REMARK	3			1CRL	21
				1CRL	22

Molecules To Go (Formerly known as Molecules R Us)

Page 2 of 3

REMARK 3 REFINEMENT. 1CRL 23
 REMARK 3 PROGRAM X-PLOR 1CRL 24
 REMARK 3 AUTHORS BRUNGER 1CRL 25
 REMARK 3 R VALUE 0.134 1CRL 26
 REMARK 3 RMSD BOND DISTANCES 0.011 ANGSTROMS 1CRL 27
 REMARK 3 RMSD BOND ANGLES 2.64 DEGREES 1CRL 28
 REMARK 4 1CRL 29
 REMARK 4 THREE N-ACETYLGLUCOSAMINE RESIDUES AT TWO SITES INCLUDED: 1CRL 30
 REMARK 4 TWO N-LINKED RESIDUES AT ASN 351; ONE N-LINKED RESIDUE AT 1CRL 31
 REMARK 4 ASN 314. 1CRL 32

SEQRES 1 534 ALA PRO THR ALA THR LEU ALA ASN GLY ASP THR ILE THR 1CRL 33
 SEQRES 2 534 GLY LEU ASN ALA ILE ILE ASN GLU ALA PHE LEU GLY ILE 1CRL 34
 SEQRES 3 534 PRO PHE ALA GLU PRO PRO VAL GLY ASN LEU ARG PHE LYS 1CRL 35
 SEQRES 4 534 ASP PRO VAL PRO TYR SER GLY SER LEU ASP GLY GLN LYS 1CRL 36
 SEQRES 5 534 PHE THR SER TYR GLY PRO SER CYS MET GLN GLN ASN PRO 1CRL 37
 SEQRES 6 534 GLU GLY THR TYR GLU GLU ASN LEU PRO LYS ALA ALA LEU 1CRL 38
 SEQRES 7 534 ASP LEU VAL MET GLN SER LYS VAL PHE GLU ALA VAL SER 1CRL 39
 SEQRES 8 534 PRO SER SER GLU ASP CYS LEU THR ILE ASN VAL VAL ARG 1CRL 40
 SEQRES 9 534 PRO PRO GLY THR LYS ALA GLY ALA ASN LEU PRO VAL MET 1CRL 41
 SEQRES 10 534 LEU TRP ILE PHE GLY GLY PHE GLU VAL GLY GLY THR 1CRL 42
 SEQRES 11 534 SER THR PHE PRO PRO ALA GLN MET ILE THR LYS SER ILE 1CRL 43
 SEQRES 12 534 ALA MET GLY LYS PRO ILE ILE HIS VAL SER VAL ASN TYR 1CRL 44
 SEQRES 13 534 ARG VAL SER SER TRP GLY PHE LEU ALA GLY ASP GLU ILE 1CRL 45
 SEQRES 14 534 LYS ALA GLU GLY SER ALA ASN ALA GLY LEU LYS ASP GLN 1CRL 46
 SEQRES 15 534 ARG LEU GLY MET GLN TRP VAL ALA ASP ASN ILE ALA ALA 1CRL 47
 SEQRES 16 534 PHE GLY GLY ASP PRO THR LYS VAL PHE GLY GLU 1CRL 48
 SEQRES 17 534 SER ALA GLY SER MET SER VAL MET CYS HIS ILE LEU TRP 1CRL 49
 SEQRES 18 534 ASN ASP GLY ASP ASN THR TYR LYS GLY LYS PRO LEU PHE 1CRL 50
 SEQRES 19 534 ARG ALA GLY ILE MET GLN SER GLY ALA MET VAL PRO SER 1CRL 51
 SEQRES 20 534 ASP ALA VAL ASP GLY ILE TYR GLY ASN GLU ILE PHE ASP 1CRL 52
 SEQRES 21 534 LEU ALA SER ASN ALA GLY CYS GLY SER ALA SER ASP 1CRL 53
 SEQRES 22 534 LYS LEU ALA CYS LEU ARG GLY VAL SER SER ASP THR LEU 1CRL 54
 SEQRES 23 534 GLU ASP ALA THR ASN ASN THR PRO GLY PHE LEU ALA TYR 1CRL 55
 SEQRES 24 534 SER SER LEU ARG LEU SER TYR LEU PRO ARG PRO ASP GLY 1CRL 56
 SEQRES 25 534 VAL ASN ILE THR ASP ASP MET TYR ALA LEU VAL ARG GLU 1CRL 57
 SEQRES 26 534 GLY LYS TYR ALA ASN ILE PRO VAL ILE ILE GLY ASP GLN 1CRL 58
 SEQRES 27 534 ASN ASP GLU GLY THR PHE GLY THR SER SER LEU ASN 1CRL 59
 SEQRES 28 534 VAL THR THR ASP ALA GLN ALA ARG GLU TYR PHE LYS GLN 1CRL 60
 SEQRES 29 534 SER PHE VAL HIS ALA SER ASP ALA GLU ILE ASP THR LEU 1CRL 61
 SEQRES 30 534 MET THR ALA TYR PRO GLY ASP ILE THR GLN GLY SER PRO 1CRL 62
 SEQRES 31 534 PHE ASP THR GLY ILE LEU ASN ALA LEU THR PRO GLN PHE 1CRL 63
 SEQRES 32 534 LYS ARG ILE SER ALA VAL LEU GLY ASP LEU GLY PHE THR 1CRL 64
 SEQRES 33 534 LEU ALA ARG ARG TYR PHE LEU ASN HIS TYR THR GLY GLY 1CRL 65
 SEQRES 34 534 THR LYS TYR SER PHE LEU SER LYS GLN LEU SER GLY LEU 1CRL 66
 SEQRES 35 534 PRO VAL LEU GLY THR PHE HIS SER ASN ASP ILE VAL PHE 1CRL 67
 SEQRES 36 534 GLN ASP TYR LEU LEU GLY SER GLY SER LEU ILE TYR ASN 1CRL 68
 SEQRES 37 534 ASN ALA PHE ILE ALA PHE ALA THR ASP LEU ASP PRO ASN 1CRL 69
 SEQRES 38 534 THR ALA GLY LEU LEU VAL LYS TRP PRO GLU TYR THR SER 1CRL 70
 SEQRES 39 534 SER SER GLN SER GLY ASN ASN LEU MET MET ILE ASN ALA 1CRL 71
 SEQRES 40 534 LEU GLY LEU TYR THR GLY LYS ASP ASN PHE ARG THR ALA 1CRL 72
 SEQRES 41 534 GLY TYR ASP ALA LEU PHE SER ASN PRO PRO SER PHE PHE 1CRL 73
 SEQRES 42 534 VAL 1CRL 74
 FTNOTE 1 1CRL 75
 FTNOTE 1 CIS PROLINE - PRO 390 1CRL 76
 HET NAG 990 14 N-ACETYL-D-GLUCOSAMINE 1CRL 77
 HET NAG 991 14 N-ACETYL-D-GLUCOSAMINE 1CRL 78
 HET NAG 994 14 N-ACETYL-D-GLUCOSAMINE 1CRL 79
 FORMUL 2 NAG 3(C8 H15 N1 O6) 1CRL 80
 FORMUL 3 HOH *310(H2 O1) 1CRL 81
 HELIX 1 H1 LEU 73 GLN 83 1 FLAP 1CRL 82

HELIX	2	H2	ALA	136	MET	145	1			1CRL	83					
HELIX	3	H3	ASP	167	GLU	172	1			1CRL	84					
HELIX	4	H4	ALA	177	ASP	191	1			1CRL	85					
HELIX	5	H5	ALA	210	LEU	220	1			1CRL	86					
HELIX	6	H6	ILE	253	ALA	266	1			1CRL	87					
HELIX	7	H7	LYS	274	ARG	279	1			1CRL	88					
HELIX	8	H8	SER	283	THR	290	1			1CRL	89					
HELIX	9	H9	ASP	318	ARG	324	1			1CRL	90					
HELIX	10	H10	THR	343	THR	347	1			1CRL	91					
HELIX	11	H11	ASP	355	SER	365	1			1CRL	92					
HELIX	12	H12	ASP	371	ALA	380	1			1CRL	93					
HELIX	13	H13	PHE	403	HIS	425	1			1CRL	94					
HELIX	14	H14	ASP	452	GLN	456	1			1CRL	95					
HELIX	15	H15	SER	464	ALA	475	1			1CRL	96					
HELIX	16	H16	THR	519	LEU	525	1			1CRL	97					
SHEET	1	BN	3	PRO	2	LEU	6	0		1CRL	98					
SHEET	2	BN	3	ASP	10	GLY	14	-1	N	GLY	14	O	PRO	2	1CRL	99
SHEET	3	BN	3	GLY	50	PHE	53	1	N	PHE	53	O	THR	13	1CRL	100
SHEET	1	BC	11	LEU	15	ALA	17	0			1CRL	101				